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TABLES FOR THE STEP-BY-STEP INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS OF THE FIRST ORDER

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By

William F. Pickard

March 25, 1963

Technical Report No. 406

Cruft Laboratory
Harvard University
Cambridge, Massachusetts

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TABLES FOR THE STEP-BY-STEP INTEGRATION OF ORDINARY DIFFERENTIAL EQUATIONS OF THE FIRST ORDER

by

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ABSTRACT

A study is made of the step-by-step integration of ordinary differential equations of the first order by means of formulas obtained from the Gregory-Newton backward interpolating formula. Tables of relevant constants are presented.

Consider the ordinary differential equation of the first order

$$y' = f(y, x) \tag{1}$$

which is to be integrated step-by-step over $x = a(h)b$. A natural method for accomplishing this integration is a predictor-corrector process based upon a suitable finite difference interpolating formula.

Let x_o be a tabular point within (a, b) and assume that y is known at the points $x_{-j} = x_o - jh$ $(j = 0, 1, \ldots, \frac{x_o - a}{h})$. One can then write for y' the approximation to it which is provided by the Gregory-Newton backward interpolating formula

$$y' = \sum_{j=0}^{J} \frac{1}{j!} (u+j-1)^{[j]} \Delta^j f_{-j} + h^{J+1} \frac{1}{(J+1)!} (u+J)^{[J+1]} \; {}^{(J+1)}(\xi) \tag{2}$$

where $u = (x - x_o)/h$, $\Delta^j f_{-j}$ is the j^{th} forward difference of y' about x_{-j}, $x_{-J} \leq \xi \leq x_o$, and $(u - \ell)^{[j]}$ is the factorial polynomial

$$(u - \ell)^{[j]} = (u - \ell)(u - \ell - 1) \cdots (u - \ell - j + 1) \tag{3}$$

which possesses the expansion

$$(u - \ell)^{[j]} = \sum_{k=0}^{j} {}_{\ell}S_k^j \, u^{j-k} \tag{3'}$$

where the ${}_{\ell}S_k^j$ are the generalized Stirling numbers of the first kind [1]. The formula (2) can be integrated in two fashions. In the first it is assumed that $y_0, y_{-1}, \ldots, y_{-J}$ are accurately known and that a prediction of $y_1 = y(x_1)$ is desired:

$$y(x_1) = y_o + h \sum_{j=0}^{J} \beta_j \, \Delta^j f_{-j} + E_J \qquad \text{PREDICTOR} \tag{4}$$

where the error E_J is given by

$$|E_J| \leq h^{J+2} \, \beta_{J+1} \, |f^{(J+1)}|_{max} \tag{5}$$

and

$$\beta_j = \frac{1}{j!} \int_o^1 (u + j - 1)^{[j]} \, du \tag{6a}$$

$$= \frac{1}{j} \sum_{p=0}^{j} \frac{1}{j+1-p} \; {}_{-(j-1)}S_p^{\,j} \tag{6b}$$

$$= \frac{\aleph_j}{L(j)\,j!} \tag{6c}$$

where $L(j)$ is the least common denominator of $1/1$, $1/2$, ..., $1/(j+1)$. In the second method it is assumed that y_{-1}, ..., y_{-J} are accurately known, that y_0 is approximately known, and that a <u>corrected</u> value of y_0 is desired:

$$y(x_o) = y_{-1} + \sum_{j=0}^{J} \beta_j^* \, \Delta^j f_{-j} + E_J^* \qquad \text{CORRECTOR} \tag{7}$$

where the error E_J^* is given by

$$|E_J^*| \leq h^{J+2} |\beta_{J+1}^*| \, |f^{(J+1)}|_{max} \tag{8}$$

Table I

$\aleph_j$, $\aleph_j^*$, and $L(j)j!$

$j \rightarrow$	0	1	2	3	4	5	6	7	8	9	10
$\aleph_j$	1	1	5	27	502	2 375	−95 435	1 287 965	29 960 476	262 426 878	28 184 365 650
$\aleph_j^*$	1	-1	-1	-3	-38	- 135	- 4 315	-48 125	- 950 684	-7 217 406	- 682 590 930
$L(j)j!$	1	2	12	72	1 440	7 200	302 400	4 233 600	101 606 400	914 457 600	100 590 336 000

and

$$\beta_j^* = \frac{1}{j!} \int_{-1}^{0} (u+j-1)^{[j]} \, du \tag{9a}$$

$$= \frac{1}{j!} \sum_{p=0}^{j} \frac{(-1)^{j-p}}{j+1-p} \; {}_{-(j-1)}S_p^{\,j} \tag{9b}$$

$$= \frac{\aleph_j^*}{L(j)\,j!} \quad . \tag{9c}$$

This corrected value of y_0 can itself be used in (7) to obtain what is presumably a still better value of y_0, and this process can be repeated indefinitely until it converges to a final value or, in bad cases, is seen to be divergent. The use of (4) to obtain an initial estimate and the repeated use of (7) to improve this value constitutes a well-known predictor-corrector process.

The quantities β_j and β_j^*, as defined by (6a) and (9a), respectively, have been described by Collatz [2] and tabulated by him for $j = 0(1)6$. The increasing use of digital machines - often in double precision - for the integration of differential equations has made a somewhat extended table of these coefficients desirable and the existence now [1] of extensive tables of the ${}_\ell S_k^{\,j}$ has made possible the simple computation from (6b) and (9b). Table I presents the results of such an extension; the table entries were checked using the recursion relation [2]

$$\beta_{j+1} = \beta_j + \beta_{j+1}^* \quad . \tag{10}$$

Figure I presents a graph of these coefficients. The β_j can be seen to fall off slowly and can be shown, from (6a), to satisfy the inequality

$$\frac{j}{j+1} \leq \frac{\beta_{j+1}}{\beta_j} < 1 \qquad j \geq 0 \tag{11a}$$

which implies that their decline is very slow indeed. The β_j^* can be seen to fall off somewhat faster; this is to be expected since, from (6a) and (9a),

$$|\beta_j^*| < \frac{\beta_j}{j-1} \qquad j \geq 2 \tag{11b}$$

These data point up the intrinsic superiorities of corrector formulas over predictor formulas: (i) that, since $|\beta_j^*| < |\beta_j|$ the series (7) converges faster than the series (4), and (ii) that, since the β_j^* decay much faster than the β_j, the buildup of computational error in the taking of successive differences will, for a given number of terms in the interpolating series, have much less effect on the final answer when a corrector formula is used.

In actual practice the calculation of the several differences is often not carried out. Instead, the differences are expanded as

$$\Delta^j f_{-j} = \sum_{p=0}^{j} \gamma_{pj} \; f_{-p} \tag{12}$$

and (4) rewritten as

$$y(x_1) = y_o + h \sum_{j=0}^{J} \sum_{p=0}^{j} \gamma_{pj} \; \beta_j \, f_{-p} + E_J \tag{13a}$$

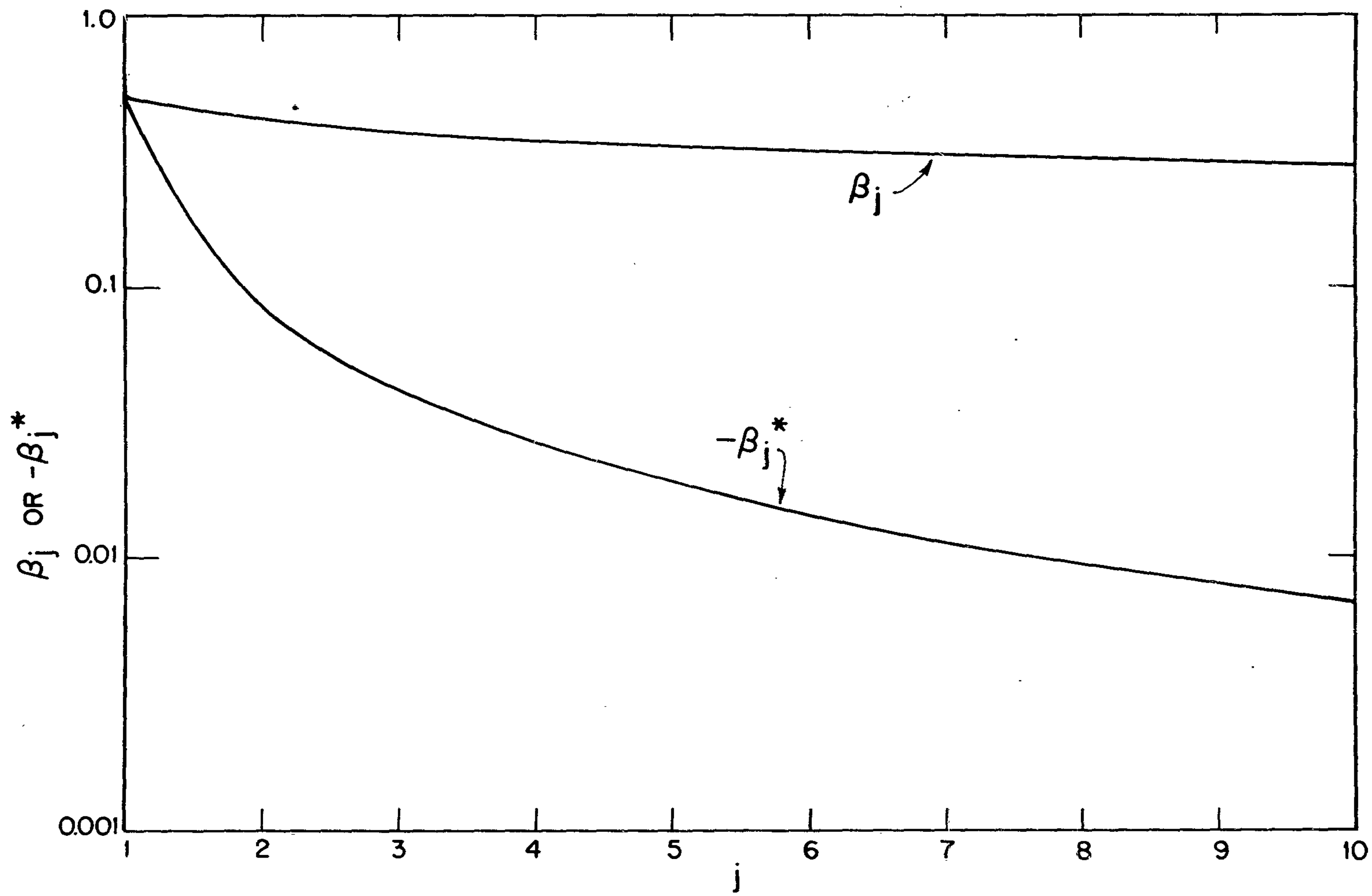

FIGURE I

TABLE II

$\delta_p(J)$

J \ p	0	1	2	3	4	5	6	7	8	9	10
0	1										
1	3	-1									
2	23	-16	5								
3	165	-177	111	-27							
4	3 802	-5 548	5 232	-2 548	502						
5	21 385	-39 615	49 910	-36 490	14 385	-2 375					
6	993 605	-2 236 440	3 527 745	-3 441 280	2 035 695	- 672 360	95 435				
7	15 198 435	-40 325 915	76 435 695	-93 256 695	73 578 505	-36 460 305	10 351 845	-1 287 965			
8	394 722 916	-1 207 505 768	2 673 350 008	-3 915 947 336	3 863 117 440	-2 552 833 976	1 087 337 608	- 270 594 968	29 960 476		
9	3 814 933 122	-13 229 393 814	33 507 517 680	-57 287 383 776	67 833 843 588	-56 041 292 412	31 829 896 224	-11 882 722 320	2 631 486 186	- 262 426 878	
10	447 827 009 070	-1 737 076 976 040	4 954 123 399 050	-9 683 736 093 360	13 380 439 581 180	-13 267 002 309 120	9 420 005 371 140	-4 689 223 333 200	1 557 759 934 710	-310 710 613 080	28 184 365 650

TABLE III

$\delta^*_p(J)$

J \ p	0	1	2	3	4	5	6	7	8	9	10
0	1										
1	1	1									
2	5	8	-1								
3	27	57	-15	3							
4	502	1 292	- 528	212	- 38						
5	2 375	7 135	-3 990	2 410	-865	135					
6	95 435	325 560	- 232 305	187 520	-101 055	31 560	-4 315				
7	1 287 965	4 894 715	-4 262 895	4 309 655	-3 099 145	1 452 465	-397 285	48 125			
8	29 960 476	125 078 632	- 128 928 632	156 670 024	- 140 927 360	88 097 464	-36 153 992	8 760 472	-950 684		
9	262 426 878	1 190 664 342	-1 420 184 304	2 016 292 320	-2 177 739 396	1 702 270 332	- 931 648 032	338 670 864	-73 512 810	7 217 406	
10	28 184 365 650	137 798 986 920	-186 936 865 290	303 703 066 800	- 382 895 428 860	359 262 650 880	-245 825 378 820	119 164 706 640	-38 803 000 950	7 619 823 960	- 682 590 930

$$= y_o + h \sum_{p=0}^{J} \alpha_p(J) f_{-p} + E_J \tag{13b}$$

$$= y_o + \frac{h}{L(J) J!} \sum_{p=0}^{J} \delta_p(J) f_{-p} + E_J \tag{13c}$$

while (7) can be rewritten as

$$y(x_o) = y_{-1} + h \sum_{j=0}^{J} \sum_{p=0}^{j} \gamma_{pj} \beta_j^* f_{-p} + E_J^* \tag{14a}$$

$$= y_{-1} + h \sum_{p=0}^{J} \alpha_p^*(J) f_{-p} + E_J^* \tag{14b}$$

$$= y_{-1} + \frac{h}{L(J) J!} \sum_{p=0}^{J} \delta_p^*(J) f_{-p} + E_J^* . \tag{14c}$$

The calculation of the next value of y can then be accomplished directly from (13c) or (14c) and the labor of maintaining a difference table thereby eliminated. Tables of $\delta_p(J)$ and $\delta_p^*(J)$ have been computed for $J = 0(1)10$ and $p = 0(1)J$ and are given in Tables II and III, respectively; they represent a considerable extension over the existing tables [2, 3] which go at most to $J = 5$*. The values of $\delta_p(J)$ and $\delta_p^*(J)$ were checked by the relations [2]

- - - - - - -

*The values of $\alpha_p(5)$ given in Reference 3 are believed to be in error.

$$1 = \sum_{p=0}^{J} \alpha_p(J) \tag{15a}$$

$$1 = \sum_{p=0}^{J} \alpha_p^*(J) \tag{15b}$$

and by having key portions of the computations individually repeated.

The selection of a predictor-corrector pair for a specific problem is by no means simple, it being necessary to choose J and h with care to minimize the effects of roundoff and truncation error. However, for modern digital machines operated in double precision, $J = 10$ will probably be as large as is profitable since by this point the computing error generated in calculating the $\Delta^i f_{-j}$ will be growing much faster than the β_j^* will be decreasing, and the total error due to this cause will normally be at least as important as the truncation error E_J^*. Finally, for suitable $f(y, x)$, it may be desirable to suspend the common practice of using a low order predictor to obtain an estimate of the next point which can then be improved using a high order corrector; the existence of high order predictors makes the initial use of a high order predictor formula and the suspension of corrector iterations seem attractive where the superior roundoff suppressing properties of a corrector formula are not essential.

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